

Methyl salicylate
119-36-8 | DTXSID5025659

Model Performance

Model

Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.91	1.08	0.91	1.08	0.92	1.00

Model Results

Predicted value: 4.27e-03 mmHg

Global applicability domain: Inside

Local applicability domain index: 7.28e-01

Confidence level: 4.09e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>4-(2,4-Dinitroanilino)phenol</div> <div>Measured: 3.43e-02</div> <div>Predicted: 1.31e-11</div>	<div>Image not found</div> <div>2-Methoxyprop-1-ene</div> <div>Measured: 8.46e-02</div> <div>Predicted: 474</div>	<div>Image not found</div> <div>2,6-Diethylaniline</div> <div>Measured: 1.59e-05</div> <div>Predicted: 2.02e-02</div>
<div>Image not found</div> <div>Butyl phenyl ether</div> <div>Measured: 1.08e-03</div> <div>Predicted: 5.92e-01</div>	<div>Image not found</div> <div>O,O-Dimethyl chlorothiophosphate</div> <div>Measured: 3.60e-04</div> <div>Predicted: 4.40e-01</div>	